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ISSN 1477-9226



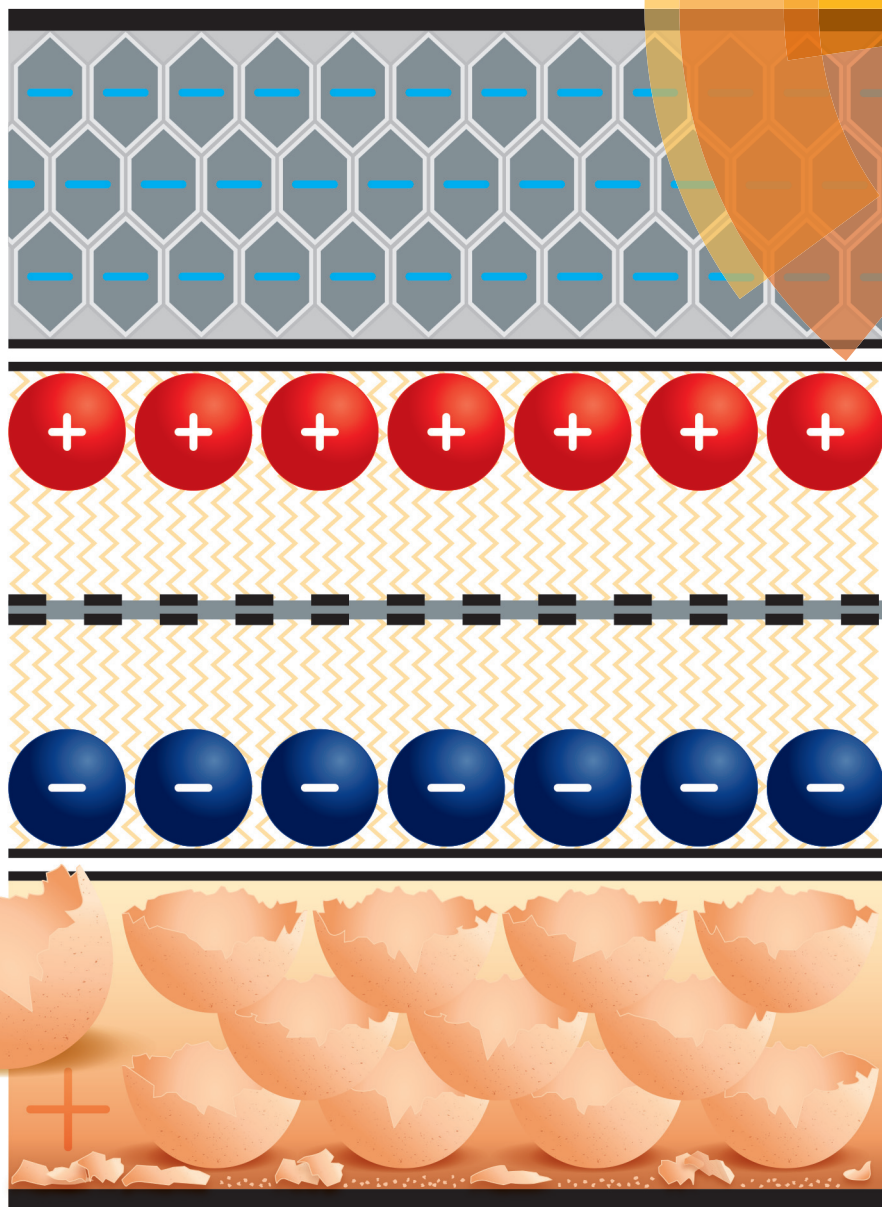
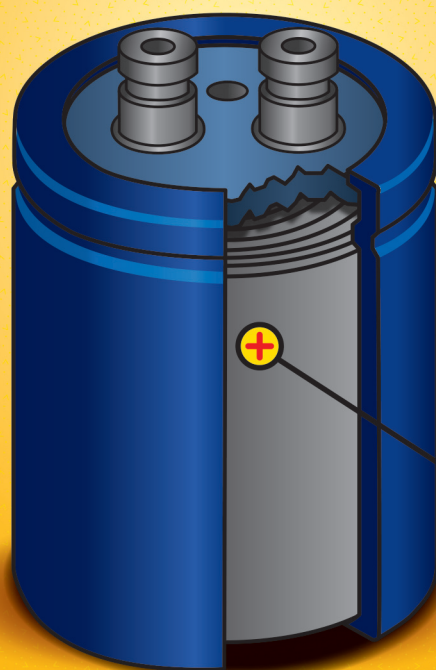
PAPER

Shen-ming Chen, Xiaoheng Liu *et al.*
One pot synthesis of α -AgVO₃/palygorskite nanocomposites with enhanced photocatalytic activity using triple roles of palygorskite: supporter, dispersant and growth-directing agent

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COMMUNICATION

Manickam Minakshi, Maximilian Fichtner *et al.*
Bio-waste chicken eggshells to store energy

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IN THIS ISSUE

ISSN 1477-9226 CODEN DTARAF 47(47) 16815–17178 (2018)



Cover

See Shen-ming Chen,
Xiaoheng Liu *et al.*,
pp. 16855–16861.

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16855.



Inside cover

See Manickam Minakshi,
Maximilian Fichtner *et al.*,
pp. 16828–16834.

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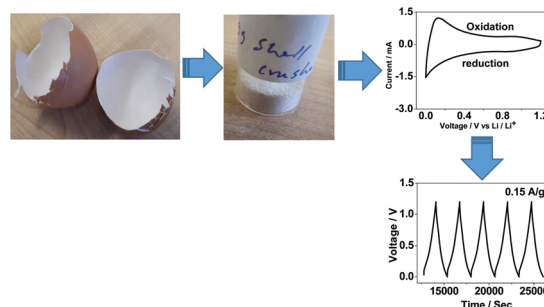
COMMUNICATIONS

16828

Bio-waste chicken eggshells to store energy

Manickam Minakshi,* Heidy Visbal, David R. G. Mitchell
and Maximilian Fichtner*

Chicken eggshell, a calcite mineral (CaCO_3) along with an
inner shell membrane, is crushed into a powder to be used
as an electrode for a lithium-ion capacitor.

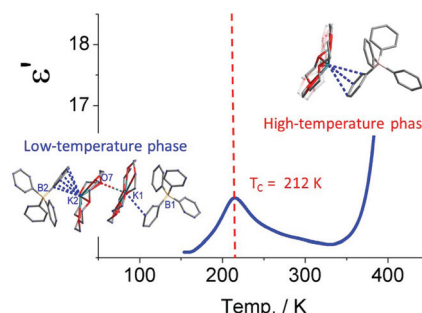


16835

An organometallic half-sandwich supramolecular complex $\{\text{K}(18\text{-Crown-6})(\eta^n\text{-C}_6\text{H}_5\text{B}(\text{C}_6\text{H}_5)_3)\}$ ($n = 1\text{--}6$) exhibiting a reversible breaking-symmetry phase transition and switchable dielectric behaviour

Guo-Jun Yuan,* Dong-Sheng Shao, Zhi-Yuan Yao,
Wen-Long Liu and Xiao-Ming Ren*

An organometallic supramolecular crystal of $\{\text{K}(18\text{-crown-6})(\eta^n\text{-C}_6\text{H}_5\text{B}(\text{C}_6\text{H}_5)_3)\}$ ($n = 1\text{--}6$) has a half-sandwich structure and exhibits a reversible breaking-symmetry phase transition and switchable dielectric behavior.



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Dalton Transactions (print: ISSN 1477-9226;
electronic: ISSN 1477-9234) is published 48 times
a year by the Royal Society of Chemistry,
Thomas Graham House, Science Park, Milton Road,
Cambridge, UK CB4 0WF.

All orders, with cheques made payable to the
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2018 Annual (print+electronic) subscription price: £4503;
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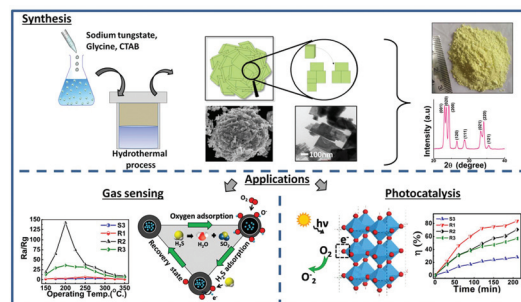
COMMUNICATIONS

16840

Ru-Loaded mesoporous WO₃ microflowers for dual applications: enhanced H₂S sensing and sunlight-driven photocatalysis

S. S. Mehta, D. Y. Nadargi, M. S. Tamboli,
L. S. Chaudhary, P. S. Patil, I. S. Mulla and
S. S. Suryavanshi*

We report a facile synthesis of Ru-loaded WO₃ marigold structures through a hydrothermal route and their bidirectional applications as enhanced H₂S gas sensors and efficient sunlight-driven photocatalysts.

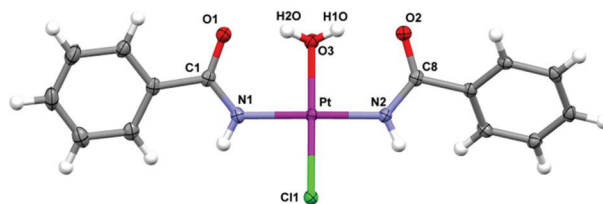


16846

Platinum-mediated monohydration of SO₂

Antonio Gimeno-Prat, Adrián Cortés-Sanchón,
Antonio Martín, Miguel Baya* and José M. Casas*

The monohydration of SO₂ has been achieved in solution mediated by a platinum-aquo complex.

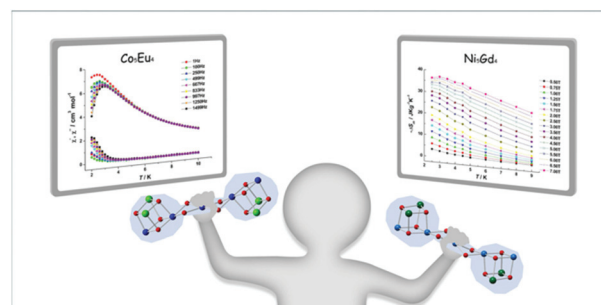


16850

Facile and environmentally friendly synthesis of six heterometallic dumbbell-shaped M₅Ln₄^{III} (M = Co, Ni; Ln = Eu, Gd, Dy) clusters as cryogenic magnetic coolants and molecular magnets

Feng Shao, Jia-Jia Zhuang, Ming-Guang Chen,
Ning Wang, Hai-Yan Shi, Jia-Ping Tong,* Gang Luo,
Jun Tao and Lan-Sun Zheng

The work demonstrates a facile and environmentally friendly synthesis of hexanuclear clusters as cryogenic magnetic coolants and molecular magnets.



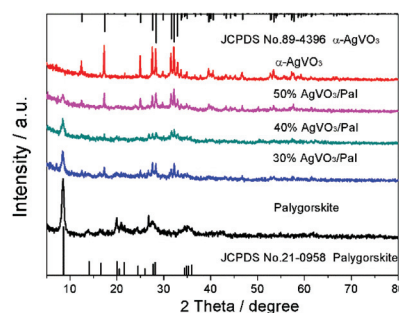
PAPERS

16855

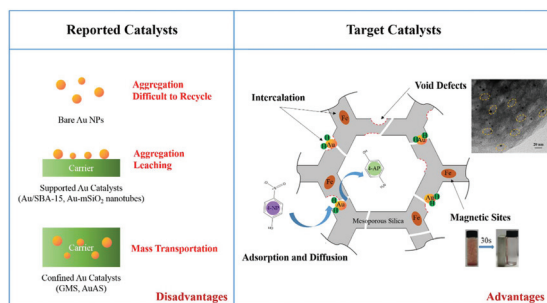
One pot synthesis of α-AgVO₃/palygorskite nanocomposites with enhanced photocatalytic activity using triple roles of palygorskite: supporter, dispersant and growth-directing agent

Yuting Luo, Jie Luo, Yuxiang Hua, Jiacheng Yao,
Shen-ming Chen* and Xiaoheng Liu*

Novel α-AgVO₃/palygorskite nanocomposites were successfully prepared via a one pot deposition precipitation method.



16862

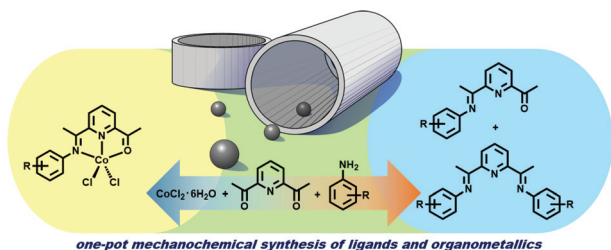


In situ intercalation of Au nanoparticles and magnetic γ -Fe₂O₃ in the walls of MCM-41 with abundant void defects for highly efficient reduction of 4-nitrophenol and organic dyes

Shijian Zhou, Weiming Jin, Yun Ding, Bo Shao, Bangbang Wang, Xu Hu and Yan Kong*

Au nanoparticles and magnetic γ -Fe₂O₃ are intercalated *in situ* in the walls of MCM-41, and abundant void defects appeared during the assembly process.

16876

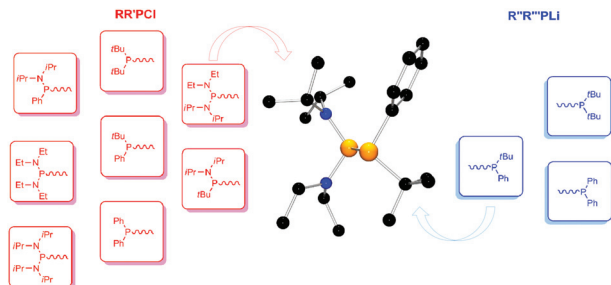


Mechanochemical routes for the synthesis of acetyl- and bis-(imino)pyridine ligands and organometallics

Thomas E. Shaw, Lorianne R. Shultz, Louiza R. Garayeva, Richard G. Blair, Bruce C. Noll and Titel Jurca*

Mechanochemical synthesis, conducted by ball milling, affords rapid access to acetyl- and bis(imino)pyridine ligands and acetyl(imino)pyridine cobalt species.

16885

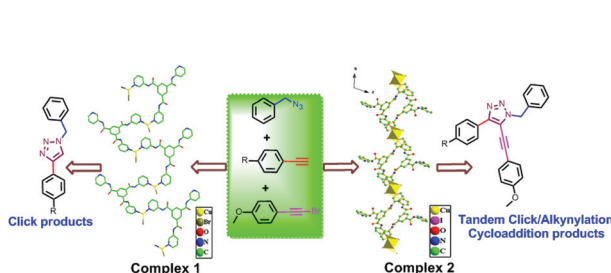


Symmetrical and unsymmetrical diphosphanes with diversified alkyl, aryl, and amino substituents

Natalia Szykiewicz, Łukasz Ponikiewski and Rafał Grubba*

Synthesis, classification, and analysis of the structural, electronic and spectroscopic properties of a series of novel diphosphanes with diversified substituents.

16895



Cu(I) coordination polymers (CPs) as tandem catalysts for three-component sequential click/alkynylation cycloaddition reaction with regiocontrol

Xiaoqing Guo, Chao Huang,* Haiyan Yang, Zhichao Shao, Kuan Gao, Na Qin, Gaoxiang Li, Jie Wu* and Hongwei Hou*

Two synthesized Cu(I)-based CPs could catalyze the three-component sequential click/alkynylation cycloaddition reaction with high regioselectivity.

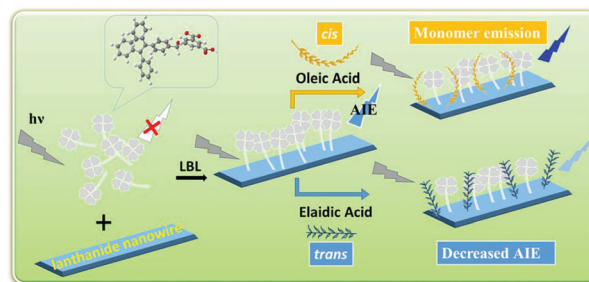
PAPERS

16902

Inducing the distinctly different fluorescence properties of a tetraphenylethene (TPE) derivative modified lanthanide nanowire upon the addition of a pair of *cis*- and *trans*-isomers of fatty acids

Jianbin Wu, Songyang Huang, Yan Gao, Jiale Li and Xi Wang*

Different fluorescence properties of a tetraphenylethene (TPE) derivative modified lanthanide nanowire were induced by a pair of *cis*- and *trans*-isomers of fatty acids.

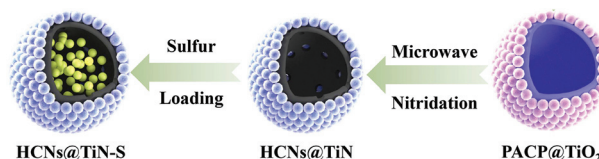


16909

Microwave-assisted rapid preparation of hollow carbon nanospheres@TiN nanoparticles for lithium–sulfur batteries

Jianxin Tu, Hejun Li, Jizhao Zou,* Shaozhong Zeng, Qi Zhang, Liang Yu and Xierong Zeng*

Hollow carbon nanospheres@TiN nanoparticles (HCNs@TiN) were designed and successfully synthesized via a microwave reduction method.

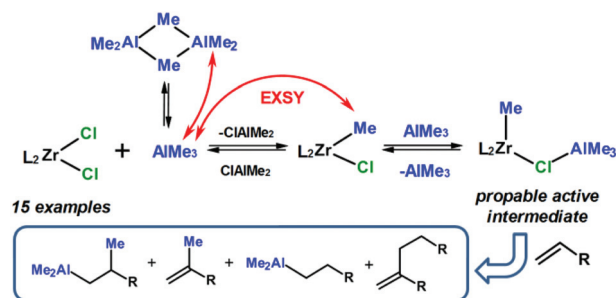


16918

Ligand exchange processes in zirconocene dichloride–trimethylaluminum bimetallic systems and their catalytic properties in reaction with alkenes

Lyudmila V. Parfenova,* Pavel V. Kovyazin, Vener Z. Gabdrakhmanov, Galina P. Istomina, Pavel V. Ivchenko, Ilya E. Nifant'ev, Leonard M. Khalilov and Usein M. Dzhemilev

The exchange processes in the system $L_2ZrCl_2-(AlMe_3)_2$ and its reactivity towards the alkene were studied.

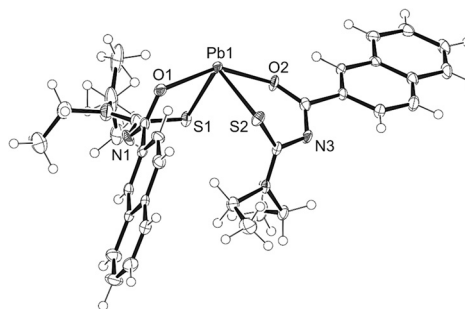


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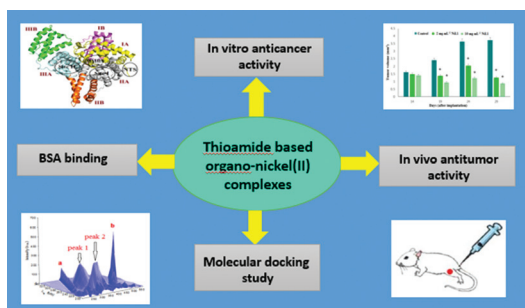
Full compositional control of PbS_xSe_{1-x} thin films by the use of acylchalcogourato lead(II) complexes as precursors for AACVD

Tagbo Emmanuel Ezenwa, Paul D. McNaughten,* James Raftery, David J. Lewis and Paul O'Brien*

Selenium and sulfur derivatives of lead(II) acylchalcogourato complexes have been used to deposit PbS_xSe_{1-x} thin films by AACVD.



16944

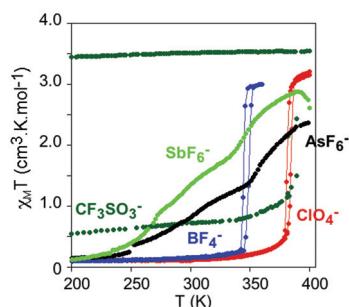


***In vitro* and *in vivo* antiproliferative activity of organo-nickel SCS-pincer complexes on estrogen responsive MCF7 and MC4L2 breast cancer cells. Effects of amine fragment substitutions on BSA binding and cytotoxicity**

M. Hosseini-Kharat,* D. Zargarian,* A. M. Alizadeh,* K. Karami, M. Saeidifar, S. Khalighfar, L. Dubrulle, M. Zakariazadeh, J.-P. Cloutier and Z. Sohrabijam

A family of organonickel complexes has been prepared, fully characterized, and tested for their antiproliferative activity against estrogen-responsive human breast cancer cells (MCF7).

16958

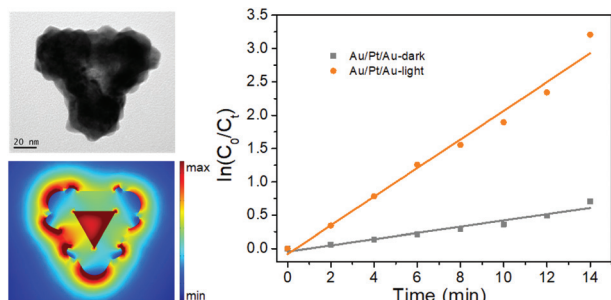


Spin-crossover compounds based on iron(II) complexes of 2,6-bis(pyrazol-1-yl)pyridine (bpp) functionalized with carboxylic acid and ethyl carboxylic acid

Víctor García-López, Mario Palacios-Corella, Alexandre Abhervé, Isaac Pellicer-Carreño, Cédric Desplanches, Miguel Clemente-León* and Eugenio Coronado*

New salts of the iron(II) bppCOOH and bppCOOEt spin crossover complexes have been studied.

16969

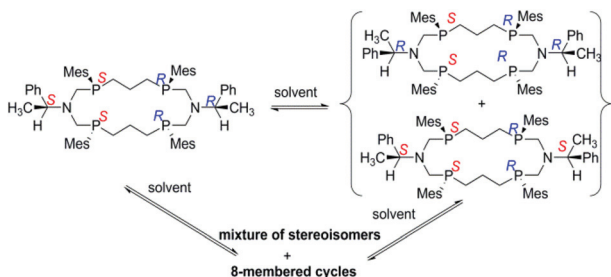


Preparation of bimetallic Au/Pt nanotriangles with tunable plasmonic properties and improved photocatalytic activity

Liang Ma,* Si-Jing Ding and Da-Jie Yang

We prepared hollow Au/Pt/Au nanotriangles with high visible light absorption, a strong tip- and center-focused local field, and superior photocatalytic activity.

16977



Chiral [16]-ane P₄N₂ macrocycles: stereoselective synthesis and unexpected intermolecular exchange of endocyclic fragments

E. I. Musina,* R. N. Naumov, K. B. Kanunnikov, A. B. Dobrynin, S. Gómez-Ruiz, P. Lönnecke, E. Hey-Hawkins, A. A. Karasik and O. G. Sinyashin

An unprecedented intermolecular exchange of endocyclic aminogroups bearing chiral substituents in "one-pot" synthesized chiral 16-membered tetrakisphosphines is discussed.

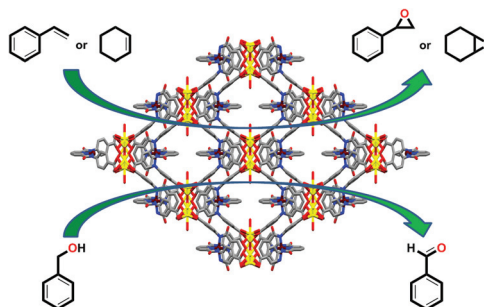
PAPERS

16985

Copper based coordination polymers based on metalloligands: utilization as heterogeneous oxidation catalysts

Gulshan Kumar, Firasat Hussain and Rajeev Gupta*

This work presents two copper-based coordination polymers and their utilization as stable, reusable and heterogeneous catalysts for the epoxidation of olefins using O_2 and for peroxide-mediated oxidation of benzyl alcohols under solvent-free conditions.

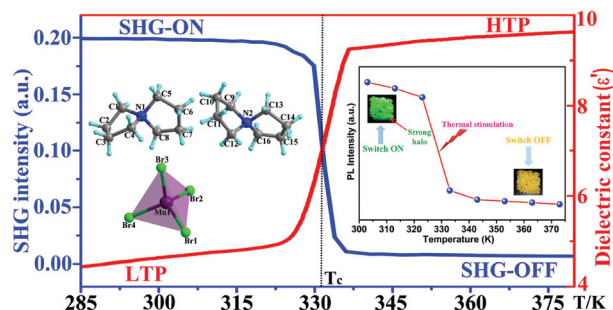


16995

A temperature-triggered triplex bistable switch in a hybrid multifunctional material: $[(CH_2)_4N(CH_2)_4]_2[MnBr_4]$

Li Xu, Ji-Xing Gao, Xiao-Gang Chen, Xiu-Ni Hua and Wei-Qiang Liao*

$[ASN]_2[MnBr_4]$ is a novel multifunctional-material-integrated compound, which simultaneously exhibits prominent dielectric/NLO/fluorescent triple switching triggered by the thermal/electric/optical signal.

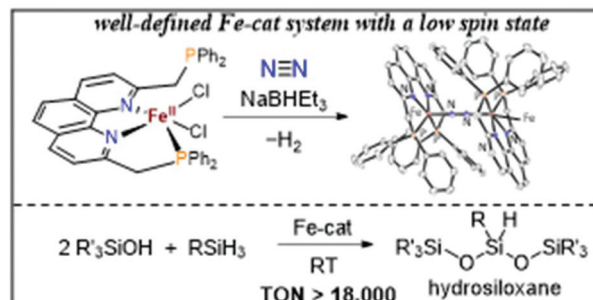


17004

Selective hydrosiloxane synthesis via dehydrogenative coupling of silanols with hydrosilanes catalysed by Fe complexes bearing a tetradentate PNNP ligand

Tomohiro Takeshita, Kazuhiko Sato and Yumiko Nakajima*

Iron complexes bearing PNNP efficiently catalyse dehydrogenative coupling of silanols with silanes to selectively form various hydrosiloxanes.

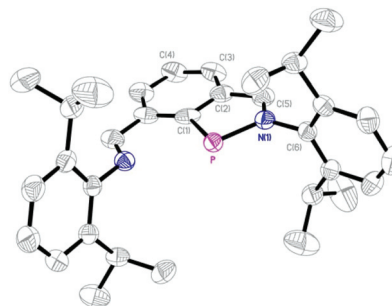


17011

Imino-stabilised phosphinidene (or azaphosphole?) and some of its derivatives

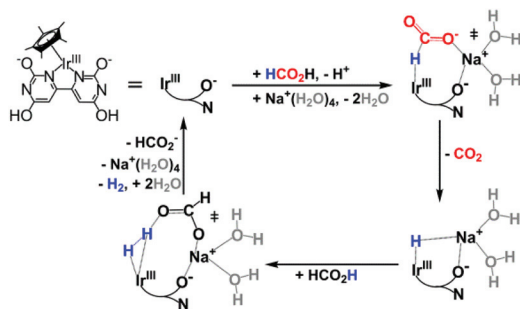
Minh Tho Nguyen, Bulat Gabidullin and Georgii I. Nikonov*

Diiminophenyl (dimph) proved to be an excellent ligand platform to stabilise a low-valent phosphorus centre.



PAPERS

17020

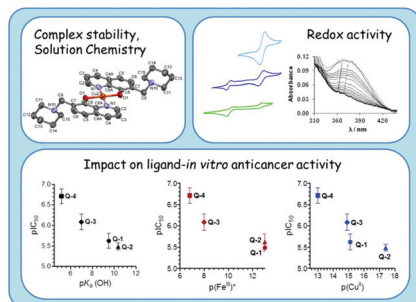


Mechanistic insights into HCO₂H dehydrogenation and CO₂ hydrogenation catalyzed by Ir(Cp*) containing tetrahydroxy bipyrimidine ligand: the role of sodium and proton shuttle

Tanakorn Wonglakhon and Panida Surawatanawong*

Catalytic HCO₂H dehydrogenation by Ir(Cp*) tetrahydroxy bipyrimidine is influenced not only by the protonation states but also by the involvement of Na⁺ and the availability of HCO₂H as a proton shuttle.

17032

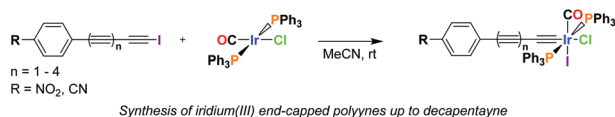


Impact of copper and iron binding properties on the anticancer activity of 8-hydroxyquinoline derived Mannich bases

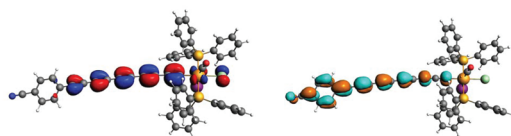
Veronika F. S. Pape, Nóra V. May, G. Tamás Gál, István Szatmári, Flóra Szeri, Ferenc Fülöp, Gergely Szakács* and Éva A. Enyedy*

A relationship between pK_a values, binding abilities to copper(II) and iron(III) and anticancer activity of 8-hydroxyquinoline derived Mannich bases.

17046



Synthesis of iridium(III) end-capped polyynes up to decapentayne



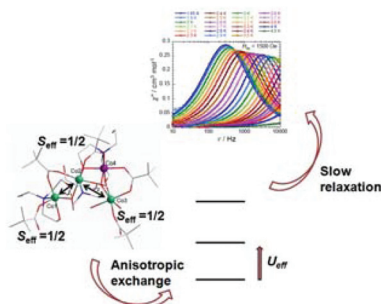
HOMO and LUMO of iridium(III) end-capped decapentayne

Selective synthesis of iridium(III) end-capped polyynes by oxidative addition of 1-iodopolyynes to Vaska's complex

Bartłomiej Pigulski, Agata Jarszak and Sławomir Szafert*

The reaction of bis(triphenylphosphine)iridium(I) carbonyl chloride (Vaska's complex) with a series of 1-iodopolyynes (1-C_nI and 2-C_nI) gave σ-polyynyl iridium(III) complexes with general formula R(C≡C)_nIr(PPh₃)₂(Cl)(I)(CO).

17055



Slow magnetization dynamics in Co(II)/Co(III) triethanolamine/pivalate complexes

Carolina Sarto, Mathieu Rouzières, Jun-Liang Liu, Heiko Bamberger, Joris van Slageren, Rodolphe Clérac and Pablo Alborés*

We report a combined computational and experimental study of SMM properties of two new pivalate cobalt complexes.

PAPERS

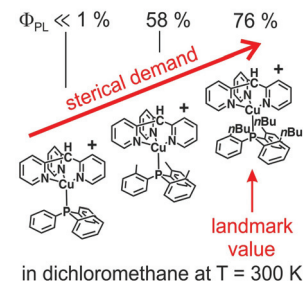
17067

Deep blue emitting Cu(I) tripod complexes. Design of high quantum yield materials showing TADF-assisted phosphorescence

Alexander Schinabeck, Nicholas Rau, Marius Klein, Jörg Sundermeyer* and Hartmut Yersin*

Triplet and singlet harvesting in combination with enhancing the emitter rigidity leads to a landmark value of the photoluminescence quantum yield for dissolved Cu(I) complexes.

TADF-assisted phosphorescence

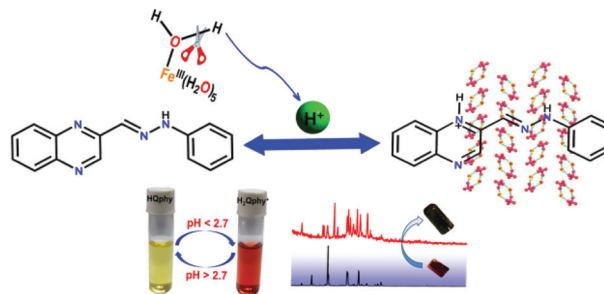


17077

A versatile quinoxaline derivative serves as a colorimetric sensor for strongly acidic pH

Riya Bag, Yeasin Sikdar, Sutapa Sahu, Dilip K. Maiti, Antonio Frontera, Antonio Bauzá, Michael G. B. Drew and Sanchita Goswami*

A strongly acidic colorimetric pH sensor induced by the acidity of [Fe(H₂O)₆]³⁺, and single crystal to single crystal transformation between the protonated and deprotonated form.

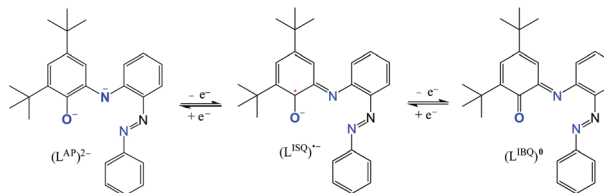


17086

Six-coordinate [Co^{III}(L)₂]^z (z = 1−, 0, 1+) complexes of an azo-appended o-aminophenolate in amidate(2−) and iminosemiquinonate π-radical (1−) redox-levels: the existence of valence-tautomerism

Amit Rajput, Anuj Kumar Sharma, Suman K. Barman, Francesc Lloret and Rabindranath Mukherjee*

Synthesis and structural (molecular and electronic) analysis for [Co^{III}{(L^{AP})(L^{ISQ})}^{3−}] (**1**, S = 1/2), [Co^{III}{(L^{ISQ})}^{2−}][PF₆]·2CH₂Cl₂ (**2**, S = 0) and [Co^{III}(η⁵-C₅H₅)₂][Co^{III}{(L^{AP})}^{2−}]₂·MeCN (**3**, S = 0) have been done.

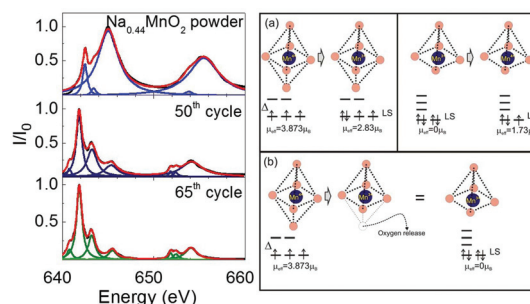


17102

Investigations of the capacity fading mechanism of Na_{0.44}MnO₂ via ex situ XAS and magnetization measurements

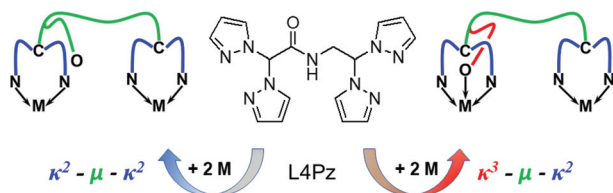
Serdar Altin*, Erdinc Oz, Emine Altin, Serkan Demirel, Ali Bayri and Sevda Avci*

We propose a capacity fading mechanism for Na_{0.44}MnO₂ via ex situ X-ray diffraction, X-ray absorption spectroscopy, Fourier transform infrared spectroscopy and magnetization measurements.



PAPERS

17109

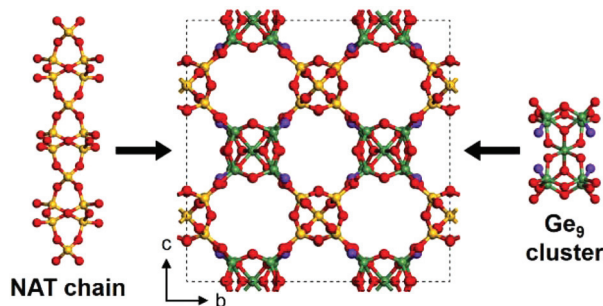


Multiple coordination modes of a new ditopic bis(pyrazolyl)methane-based ligand

John B. Coulton, Aramis C. Smith, Kraig A. Wheeler and Radu F. Semeniuc*

A new ditopic bis(pyrazolyl)methane ligand can coordinate to two metallic centers in either a $\kappa^2-\mu-\kappa^2$ or a $\kappa^3-\mu-\kappa^2$ mode.

17122

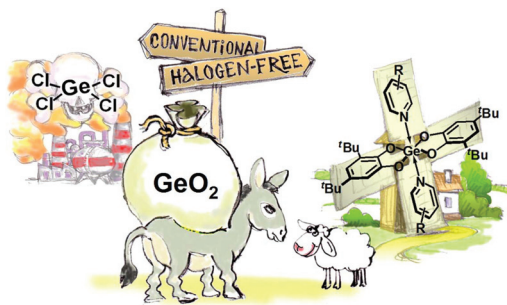


An open-framework silicogermanate regularly constructed from natrolite zeolite chains and $\text{Ge}_9\text{O}_{18}(\text{OH})_4$ clusters

Donghui Jo, Wanuk Choi, Jiho Shin and Suk Bong Hong*

An open-framework silicogermanate denoted as PST-18, whose structure is built from the natrolite chain and the Ge_9 cluster, has been synthesized.

17127

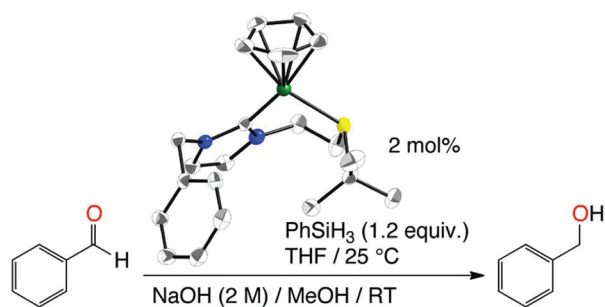


Halogen-free GeO_2 conversion: electrochemical reduction vs. complexation in $(\text{DTBC})_2\text{Ge}[\text{Py}(\text{CN})_n]$ ($n = 0 \dots 2$) complexes

Elena N. Nikolaevskaya, Evgeniya A. Saverina, Alyona A. Starikova, Amel Farhati, Mikhail A. Kiskin, Mikhail A. Syroeshkin,* Mikhail P. Egorov and Viatcheslav V. Jouikov*

3,5-di-*tert*-Butylcatecholate (DTBC) germanium complexes $(\text{DTBC})_2\text{Ge}[\text{Py}(\text{CN})_n]_2$ ($n = 0 \dots 2$) have been synthesized from GeO_2 , DTBC and $\text{Py}(\text{CN})_n$.

17134



Synthesis, characterization, and catalytic application in aldehyde hydrosilylation of half-sandwich nickel complexes bearing $(\kappa^1\text{-C})$ - and hemilabile $(\kappa^2\text{-C,S})$ -thioether-functionalised NHC ligands

Franck Ulm, Amalia I. Poblador-Bahamonde, Sabine Choppin, Stéphane Bellemin-Laponnaz, Michael J. Chetcuti,* Thierry Achard* and Vincent Ritleng*

Ni complexes bearing thioether-functionalised NHCs; hemilabile ligands for catalytic aldehyde hydrosilylation.

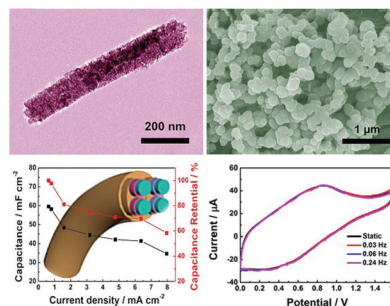
PAPERS

17146

A high performance asymmetric supercapacitor based on *in situ* prepared CuCo_2O_4 nanowires and PPy nanoparticles on a two-ply carbon nanotube yarn

X. Liang, Q. Wang,* Y. Ma and D. Zhang*

A two-ply CNT yarn asymmetric supercapacitor was fabricated by assembling a CuCo_2O_4 nanowire positive electrode and a PPy nanoparticle negative electrode. The full cell exhibits a high specific capacitance of 59.55 mF cm^{-2} and a high energy density of $0.02 \text{ mW h cm}^{-2}$.

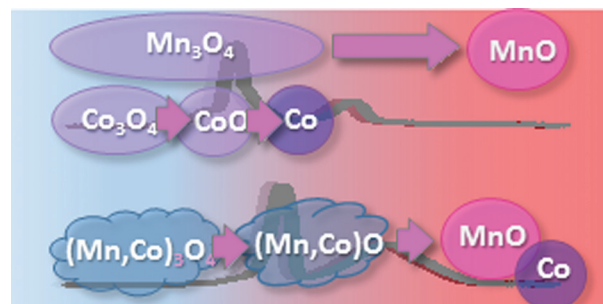


17153

Reduction of double manganese–cobalt oxides: *in situ* XRD and TPR study

Olga A. Bulavchenko,* Evgeny. Y. Gerasimov and Tatyana N. Afonassenko

The mechanism of reduction of double Mn–Co oxides with hydrogen differs significantly from the processes occurring on simple oxides.



17160

Strategic synthesis of $[\text{Cu}_2]$, $[\text{Cu}_4]$ and $[\text{Cu}_5]$ complexes: inhibition and triggering of ligand arm hydrolysis and self-aggregation by chosen ancillary bridges

Manisha Das, Angelos B. Canaj, Valerio Bertolasi, Mark Murrie and Debashis Ray*

A new family of Cu^{II} -based coordination aggregates is synthesized from HL1 with $\text{Cu}(\text{ClO}_4)_2 \cdot 6\text{H}_2\text{O}$ in the absence and presence of a group of carboxylates.

